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UPGRADE OF FASCODE AND MODTRAN TO FULL SOLAR CAPABILITY INCLUDING MULTIPLE SCATTERING AND SPHERICAL GEOMETRY

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13. ABSTRACT *(Maximum 200 words)*

A comprehensive radiative transfer algorithm (DISORT) has been interfaced with MODTRAN to provide rigorous treatment of multiple scattering. The single scattering contribution to the source-function, computed in MODTRAN, is combined with the azimuthally-averaged multiple scattering contribution from DISORT. Integration along the line-of-sight yields the intensity in any desired direction. This approach ignores the multiple scattering contribution to the azimuth-dependence of the intensity, which is important in the solar part of the spectrum. Since DISORT efficiently computes fluxes and mean intensities, the merged code facilitates the computation of fluxes, warming/cooling rates and photolysis rates.

A merged version of DISORT and FASCODE is accomplished in which the gaseous optical depths computed in FASCODE are interpolated to the same frequency step size in all layers. Compared to the original FASCODE, this merged package is computationally slower because it employs "fixed-frequency" sampling. The computational speed must be weighed against the amount of information each code produces. Whereas, FASCODE must be executed repeatedly for each new path and viewing direction, the merged FASCODE/DISORT package yields information at all desired locations and directions in a single run. The merged package provides a testbed for "benchmark" computations against which more efficient approaches may be tested.

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Contents

1. Introduction

1.1. General Objective and Philosophy

The general objective of this report is to document and discuss an upgrade of the radiative transfer code MODTRAN to include rigorous multiple scattering. Progress on work aimed at a similar upgrade for the line-by-line code FASCODE will also be discussed. For MODTRAN the upgrade is accomplished by incorporating the DISORT (DIScrete Ordinate Radiative Transfer) multiple scattering program into MODTRAN, including proper interfaces, to allow for accurate computation of multiple scattering effects. The merging of MODTRAN and DISORT is greatly facilitated by the fact that MODTRAN is a "quasi-monochromatic" code, since DISORT requires "fixed frequency" input. The heart of MODTRAN is a narrow-band model that computes gaseous path transmittances from the HITRAN data base with wavenumber steps at 1 cm^{-1}. Effective optical depths and appropriate particulate scattering parameters (also computed in the MODTRAN code) may then be input into the DISORT code which can do the complete radiative transfer computation including multiple scattering. However, the current version of DISORT is plane-parallel, whereas MODTRAN includes a geometry package that allows accurate computation of single scattering in spherical geometry. Therefore, the present implementation of DISORT into MODTRAN uses DISORT to compute only the multiple scattering component of the source function in much the same way that the present approximate multiple scattering treatments are used in MODTRAN. This approach facilitates the interfacing of DISORT with MODTRAN to provide a rigorous treatment of multiple scattering effects, and it requires only minor changes to the existing MODTRAN structure as discussed below.

In contrast to MODTRAN which is a "fixed frequency" or "quasi-monochromatic" narrow-band model, FASCODE is truly monochromatic in the sense that it is a line-by-line code. In applications of line-by-line codes to atmospheric situations one is faced with the problem that lines are pressure-broadened at low altitudes (for which a Lorentz profile is adequate), while they become Doppler-broadened at high altitudes. To optimize computational efficiency, FASCODE employs a different wavenumber step size at individual atmospheric layers, depending on the local temperature, pressure and line half-width. Interpolation is then used to connect the absorptance at a particular wavenumber

across the atmospheric layers. Thus, although FASCODE may be considered to be truly monochromatic, it is not "fixed frequency", and is therefore not automatically compatible with the DISORT multiple scattering algorithm which requires "fixed frequency" input. One way to make FASCODE compatible with DISORT is to use an interpolation scheme to interpolate optical depth to "fixed frequency" steps. The advantage of this procedure is that it would also provide a framework within which "benchmark" line-by-line multiple scattering computations could be accomplished with the combination of FASCODE and DISORT. Such a benchmark constitutes a necessary step towards the development of an ultimate line-by-line radiative transfer code with rigorous multiple scattering and optimum frequency sampling. The disadvantage of such a "benchmark" computation is that it is expensive, because it does not employ a flexible frequency sampling strategy to optimize the computational speed. On the other hand, it is relatively easy to implement, and does not require extensive bookkeeping and storage requirements (which are also computationally expensive) such as those in the current implementation of multiple scattering in FASCODE based on the adding approach (Isaacs et al., 1986).

1.2. Advantages of Merged Package

There are several advantages of merging MODTRAN and FASCODE with DISORT:

- accurate multiple scattering computations are important in the shortwave region (i.e., Rayleigh scattering) for clear sky conditions, and even more important in the presence of aerosols and clouds across the solar spectrum;
- in the terrestrial infrared part of the spectrum (e.g., beyond 4 μm) molecular (Rayleigh) scattering is negligible, but multiple scattering from aerosol and cloud particles can not be ignored and should be included;
- solar capability would become available in FASCODE which currently does not have such capability.

Hence, the improved treatments of multiple scattering in the merged MODTRAN/ FASCODE and DISORT packages would provide valuable research tools for a variety of applications.

1.3 Scope of Work

This document is organized as follows. We start with a brief description of MODTRAN and FASCODE outlining their strengths as well as their weaknesses to motivate the usefulness of the merging described here. This is followed by a brief summary of the general-purpose multiple scattering algorithm called DISORT. Next, we discuss the interfacing of DISORT with MODTRAN and FASCODE. Validation of the merged packages is the subject of Section 4 where we provide sample comparisons of computational results from the original MODTRAN and FASCODE programs and from the merged packages. A more comprehensive validation of the merged MODTRAN/DISORT package is provided in the Appendix. A discussion of future improvements of the merged MODTRAN/DISORT package as well as a possible approach for enhancing the merging of FASCODE with DISORT is provided in Section 5. Finally, a summary is given in Section 6.

2. Brief Description of MODTRAN and FASCODE

Planning the design and deployment of communication and remote sensing equipment require the development of accurate models to predict adverse environmental effects upon the devices. For this reason, the Phillips Laboratory (previously known as the Air Force Geophysical Laboratory) developed the radiative transfer model LOWTRAN (Selby et al., 1978; Kneizys et al., 1983). The original version of LOWTRAN did not include multiple scattering; approximate treatment of multiple scattering was added at a later stage (Isaacs et al., 1986; Isaacs et al., 1987). Since the development of these first versions of LOWTRAN, numerous later versions have appeared. Each of these newer version has included additional options and improvements in physics and modeling (Kneizys et al., 1988).

The most modern version of these models produced by the Phillips Laboratory is known as "The Moderate Resolution Model for LOWTRAN 7", which is commonly referred to as MODTRAN (Berk et al., 1989). At present, MODTRAN constitutes the most advanced band model for the computation of atmospheric transmittance and radiance. Its spectral range is from 0 to 50,000 cm^{-1} (0.2 μm to infinity), and the spectral resolution ranges from 50 cm^{-1} to 2 cm^{-1} (Berk et al., 1989). As in the earlier version of LOWTRAN, the latest version of MODTRAN (MODTRAN2) has retained all of the capabilities of the older versions. One

important aspect of MODTRAN is that band model parameters are taken directly from the HITRAN data base for the twelve atmospheric molecules considered in the model: $H_2O, CO_2, O_3, N_2O, CO, CH_4, O_2$, NO, SO_2, NO_2, NH_3, HNO_3 (Kneizys et al., 1988).

FASCODE (Fast Atmospheric Signature Code) is a line-by-line code that was specifically designed to improve the efficiency of line-by-line computations (Smith et al., 1978). It is essentially an algorithm for the reconstruction of the Voigt line profile within 64 half-widths of a given wave number for a constant atmospheric temperature, pressure and composition. A key feature of FASCODE is the decomposition of the Voigt profile into four functions, one of which is Gaussian used to represent the Doppler core of the line out to 4 half-widths, while the remaining three functions approximate the Lorentz wings of the line. This decomposition allows the rapidly varying portion of the profile near the line center to be properly sampled by a denser grid than the more slowly varying wings of the profile which can be adequately sampled with a much coarser grid. A criterion for optimum sampling that provides an accuracy of about 0.1% is to use a sampling interval that is one-quarter of the average half-width of the line over the frequency range of interest (Clough et al., 1977).

The extension to non-uniform atmospheric paths with varying temperature, pressure and absorber concentration is done by approximating the real atmosphere by a series of homogeneous layers in which the parameters are taken to be constant in each layer, but are allowed to vary from layer to layer. Since the pressure decreases exponentially with altitude, the average half-width and therefore the sampling interval (one-quarter of the average half-width) is larger at lower than at higher levels in the atmosphere. The absorption coefficient for each layer is then merged with those from neighboring layers in such a way that the absorptance for a path through two adjacent layers has the resolution of the higher layer by interpolating the coarser resolution results for the lower layer into the fine resolution of the higher layer. In FASCODE this procedure is executed in a systematic manner so that the spectral absorptance for a given atmospheric slant path is obtained with the finest spectral resolution (defined by the sampling criterion for the highest level) at all atmospheric levels. The transmittance between any two boundaries may now be computed, and used to obtain the radiance along a given path usually assuming (but not limited to) local thermodynamic equilibrium (LTE) so that the emission is given

by the Planck function depending exclusively on frequency and temperature. For completeness we note that FASCODE does possess full NLTE capability.

The original version of FASCODE (Smith et al., 1978) treated particle scattering as equivalent to absorption so that all scattered radiation is re-emitted as if it were absorbed. An approximate treatment of multiple scattering was introduced by Isaacs et al. (1986) using a two-stream approximation combined with an adding algorithm. The adding method was chosen because it is consistent with the radiance/ transmittance computation in FASCODE which treats one layer at the time. This approach is efficient because it allows for an optimum sampling strategy in which the resolution in a given layer is determined by the line half-width in that layer, but is inconsistent with monochromatic multiple scattering treatments which require the use of a fixed frequency throughout the atmosphere. From a computational point of view the main advantage of this approach is that the multiple scattering computations will not have to be done at the finest spectral resolution except in the highest atmospheric layer of interest. In layers below, the coarser spectral resolution implies that significant savings in computing time are obtained by this approach.

In the absence of scattering only the layers included in the atmospheric path under consideration need to be considered in the radiance computation. However, the presence of multiple scattering necessitates the consideration of all layers containing scattering material, including layers above and below those defined by the atmospheric path of interest. This requirement not only increases the computational time, but also complicates the bookkeeping considerably. For example, in an atmosphere with tropospheric and stratospheric aerosols, scattering may be important in most atmospheric layers. Thus, even though the radiance may be desired only for a path from say 2 to 4 km, multiple scattering computations are needed for all layers containing scattering particles above and below this altitude range. Typically this extra computational effort results in an increase in CPU execution time for FASCODE runs with multiple scattering by a factor 3-4 over a standard run in which multiple scattering is ignored. It is interesting to note that most of this additional time is due to the required spectral merging of stored quantities rather than multiple scattering computations (Isaacs et al., 1986). In addition, multiple scattering runs of FASCODE require three times the storage space of standard runs without multiple scattering. Thus, although the adding-approach

to implement multiple scattering in FASCODE is consistent with existing code structure and frequency sampling strategy, it is quite cumbersome to implement and implies a factor of 3 or so increase in computational effort and storage requirement due to spectral merging in addition to the cost of the multiple scattering computations. This is an important fact to keep in mind when considering alternative approaches that would allow for more accurate treatment of multiple scattering in FASCODE.

Several atmospheric models are available in MODTRAN and FASCODE including tropical, midlatitude summer, midlatitude winter, subarctic winter, subarctic summer, and the 1976 U. S. standard atmosphere (Anderson et al., 1986). A user-specified atmospheric model may also be adopted (e.g., from radiosonde data). In addition, both MODTRAN and FASCODE have haze and volcanic aerosol models as well as cloud models which may be used in conjunction with the model atmospheres described above (Shettle 1989).

From the point of view of working with the MODTRAN and FASCODE codes, they have one major disadvantage: there is a general lack of documentation within the codes that make them difficult to read and understand. Due to the volume of historic coding required in the development of MODTRAN and FASCODE many programmers have been involved. This has led to a variety of programming styles appearing throughout the code. MODTRAN and FASCODE consist of a combination of numerous subroutines and functions which are loosely linked together by common block statements. This combination of insufficient documentation, different programming styles, and common block usage makes attempts to understand and modify these computer programs a highly time-consuming and difficult task.

From the physical point of view MODTRAN and FASCODE have a more important shortcoming: multiple scattering is computed in an approximate manner using a two-stream approximation. The main purpose of the present work is to remove this shortcoming by incorporating a better multiple scattering computation in MODTRAN and FASCODE. As a side benefit, the merging of MODTRAN and FASCODE with the advanced radiative transfer algorithm DISORT provides additional capabilities that are useful for a variety of applications as already mentioned in Section 1.

3. Brief Description of DISORT

In 1988 a state-of-the-art, user-friendly discrete ordinate algorithm for radiative transfer in vertically inhomogeneous, non-isothermal, plane-parallel media was made generally available to interested users (Stamnes et al., 1988). The physical processes included in this multi-purpose algorithm are thermal emission, scattering, absorption, and reflection at the lower boundary (with any angular dependence, not only Lambertian). The system may be driven by parallel or diffuse radiation incident at the top boundary, as well as by internal thermal sources and thermal emission from the boundaries. The FORTRAN code is well-documented and well-tested. It offers an efficient and numerically stable computational scheme that lends itself readily to the solution of a variety of radiative transfer problems. The DISORT algorithm has the following unique features:

- it is unconditionally stable for an arbitrary number of quadrature angles (streams) and arbitrarily large individual layer and total optical depths;
- it may be forced by any combination of parallel beam or diffuse incidence and thermal sources in the medium and at the boundaries;
- it allows for an arbitrary bidirectional reflectivity at the lower boundary;
- it can be used to compute intensities at arbitrary angles and optical depths;
- it can be used to compute fluxes and mean intensities reliably and efficiently (by executing the code in the two- or four-stream mode) at arbitrary (user-desired) optical depths;
- it has been thoroughly tested against a wide variety of published solutions;
- unlike the popular doubling method, computing time for individual layers is independent of optical thickness; the computing time is directly proportional to the number of layers;
- the code is thoroughly documented with extensive references to published equation numbers.

It should be noted, however, that DISORT is a plane-parallel code that can only employ a spherically refractive atmosphere as supplied by an external algorithm (such as the geometry package in MODTRAN). In the present application we have interfaced the DISORT code with MODTRAN and used it to compute the multiple scattering contribution to the source function required by MODTRAN as discussed

in more detail below. A similar interfacing of DISORT with FASCODE has also been accomplished to create a benchmark line-by-line code with rigorous multiple scattering. However, more work may be needed to make the merged version of FASCODE and DISORT an efficient tool for multiple scattering computations.

4. Merging of DISORT with MODTRAN and FASCODE

4.1 DISORT/MODTRAN Merging and Validation

MODTRAN is designed to compute the intensity (or radiance) in a particular viewing direction. This can be done by direct integration along the line-of-sight of the "source function" which describes the source of radiance emanating from a small volume element at a particular location in the atmosphere. In the absence of multiple scattering this source function is independent of the intensity that we are seeking and it can be computed directly as explained below. When multiple scattering effects are important the problem is considerably more complicated because then the source function does indeed depend on the intensity that we are seeking. In general, we want to solve the radiative transfer equation for the intensity, I

$$\mu \frac{dI(\tau,\mu,\phi)}{d\tau} = I(\tau,\mu,\phi) - S(\tau,\mu,\phi) \tag{1}$$

where $\mu = \cos(\theta)$; θ is the polar angle; ϕ is the azimuthal angle and τ the optical depth. The source function $S(\tau,\mu,\phi)$ is given by

$$S(\tau,\mu,\phi) = \frac{\omega(\tau)}{4\pi}\int_0^{2\pi} d\phi' \int_{-1}^{1} d\mu' \, P(\tau,\mu,\phi;\mu',\phi')\, I(\tau,\mu',\phi') + [1-\omega(\tau)]\, B[T(\tau)] + \frac{\omega(\tau)\, I^{inc}}{4\pi} P(\tau,\mu,\phi;-\mu_0,\phi_0)\, e^{-ch(\tau,\mu_0)} \tag{2}$$

where $\omega(\tau)$ is the single scattering albedo, P is the phase function, $B(T)$ the Planck function at temperature T, and I^{inc} the beam of radiation incident at solar zenith angle θ_0 with $\mu_0 = \cos(\theta_0)$. In equation (2) the first term represents the multiple scattering (MS) contribution to the source function, the second term is the contribution from thermal emission (TE) and the third term is the contribution due to single scattering (SS). In plane geometry $ch(\tau,\mu_0) = \tau/\mu_0 = \tau/\cos(\theta_0)$; otherwise $ch(\tau,\mu_0)$ is the actual optical path length through a curved atmosphere, including

refraction effects, which we may generically refer to as the Chapman function. This function is computed in MODTRAN's geometry routines.

In the absence of multiple scattering (when the integral term in equation (2) is ignored) the source function may be computed directly from the known temperature, T, solar beam, I^{inc}, single scattering albedo, $\omega(\tau)$, and the phase function, $P(\tau, \mu, \phi; \mu', \phi')$. It is then a simple matter to integrate equation (2) directly (using an integrating factor) to determine the intensity, I, in the desired viewing direction, θ, or $\mu = \cos(\theta)$. For situations in which scattering cannot be ignored the integral term in equation (2) must be retained and we see that the source function depends on the intensity for which we want to solve. This represents an "enormous" complication compared to the previous case in which multiple scattering was ignored. An approximate solution to equation (1) may now be used to determine the intensity, I, and thereby an approximate solution to $S(\tau,\mu,\phi)$ in equation (2). This approximate solution for S may in turn be substituted into equation (1) which may then be solved directly using again an integrating factor as explained above for the case in which multiple scattering was ignored. The accuracy of the solution will, however, depend on how accurately we determined $S(\tau,\mu,\phi)$. In DISORT this approach is used to solve for the intensity at arbitrary "viewing" angles and depths.

MODTRAN already computes quite accurately the SS term including curvature and refraction effects. The TE term is computed in MODTRAN by assuming that the temperature is isothermal within each layer, but allowed to vary from layer to layer. The MS flux is currently computed in subroutine BMFLUX using the two-stream and isothermal layer temperature approximations to solve for upward and downward fluxes which are then converted into hemispherical intensities. This is accomplished by assuming that the intensity is uniform in each hemisphere so that the hemispherical intensity is obtained from the hemispherical flux by simply dividing it by π (Isaacs et al., 1987). DISORT can compute the MS term to very high accuracy using a multi-stream approximation. To improve the accuracy of the multiple scattering computation in MODTRAN we use DISORT to compute the MS term. This implies that the quantities of solar and thermal source functions which are now based on fluxes from subroutine BMFLUX will be based on output

from DISORT.

Having studied carefully the treatment of multiple scattering in MODTRAN, we find that this approach is relatively simple to implement numerically, at least in principle. However, we note that it will not allow us to compute the azimuthal dependence of the intensity; only the azimuthally-averaged intensity will be available. For thermal infrared radiation this is no problem, since there is no azimuth-dependence. For solar radiation azimuth-dependence will be important for viewing directions other than zenith and nadir. For single scattering the azimuthal dependence is already computed in MODTRAN.

The existing DISORT program does not compute the source function *per se;* only the intensity involving an integration of the complete source function is computed. To implement this approach we have therefore written two specific subroutines in DISORT to compute the multiple scattering source function separately for solar and thermal sources as mandated by MODTRAN. Several existing subroutines are also modified slightly to adopt these changes. These two subroutines are designed to solve for the azimuthally-averaged source function (solar and thermal)

$$S(\tau,\mu) = \sum_{\substack{j=-N \\ j\neq 0}}^{N} C_j G_j(\mu) e^{-k_j \tau} + (V_0 + V_1 \tau) \tag{3}$$

where all the coefficients are computed in DISORT. We note that once these coefficients have been determined, equation (3) provides a simple analytic expression for evaluating the source function at arbitrary "viewing" angles and depths. The single scattering contribution to the source function and the thermal emission term are not included in equation (3), because our aim here is to compute the multiple scattering source function (which by definition does not contain these terms) for use in MODTRAN. In addition, depending on whether we are interested in wavelengths in the solar or thermal part of the spectrum, the source function will be non-negligible for only one of the two. Thus, for wavelengths shortward of 2 μm, the thermal radiation is small compared to the solar contribution (during daytime), whereas the solar contribution is small compared to the thermal for wavelengths longward of 5 μm. Only in the region between 2 and 5 μm do we usually need to consider both thermal and solar contributions. Therefore, to save computing resources, it would be useful to implement a switch in MODTRAN so that only the desired (non-negligible) component is computed. Of course, for the

overlap region (2 - 5 μm) where both solar and thermal radiation contribute, we must allow for the possibility of including both components.

The expression for the source function as given in equation (3) looks deceivingly simple. To implement it numerically within the existing DISORT code requires great care, due to the size and complexity of this multi-purpose code. The implementation, debugging and testing of these particular subroutines are now complete. One necessary test which we have performed is that for isotropic scattering the mean intensity (which is standard output from the subroutine FLUXES in DISORT) differs from the source function only by a factor equal to the single scattering albedo (ω). We have also tested that MODTRAN and DISORT (which can compute the full intensity including multiple and single scattering as well as thermal sources) yield essentially the same results.

A comparison of multiple scattering (MS) source functions in the ultraviolet region between 300 and 400 nm is shown in Figure 1 for a clear subarctic winter atmosphere (Anderson et al., 1986) which has layering structure of layer-1 for the lowest atmospheric layer and layer-32 for the highest. For this computation, the solar zenith angle is 25° and the viewing direction corresponds to an observer located at 100 km looking downward at 50° off nadir. The azimuth angle is set at the principal plane to maximize the scattering signature. The 16-stream DISORT results are considered as "benchmark", since all calculations (2- to 16-stream) for clear sky with Rayleigh scattering and ozone absorption have converged.

As shown in Figure 1, there is good agreement between results from MODTRAN (hereafter M2) and DISORT using 2-stream (not shown), but M2 yields smaller values at all three atmospheric layers than accurate 16-stream results (hereafter D16), and it significantly underestimates the source function for wavelengths longer than 350 nm. The absolute errors are small when the ozone absorption is the strongest (e.g., UV-B band) and increase with decreasing ozone absorption. The total spectral bi-directional radiance for this case is shown in Figure 2a, and the error as compared to the D16 results in Figure 2b. Note that the relative errors range from +5% to -17%, with a peak at wavelength about 340 nm. A more comprehensive validation of the merged MODTRAN/DISORT package is provided in the Appendix.

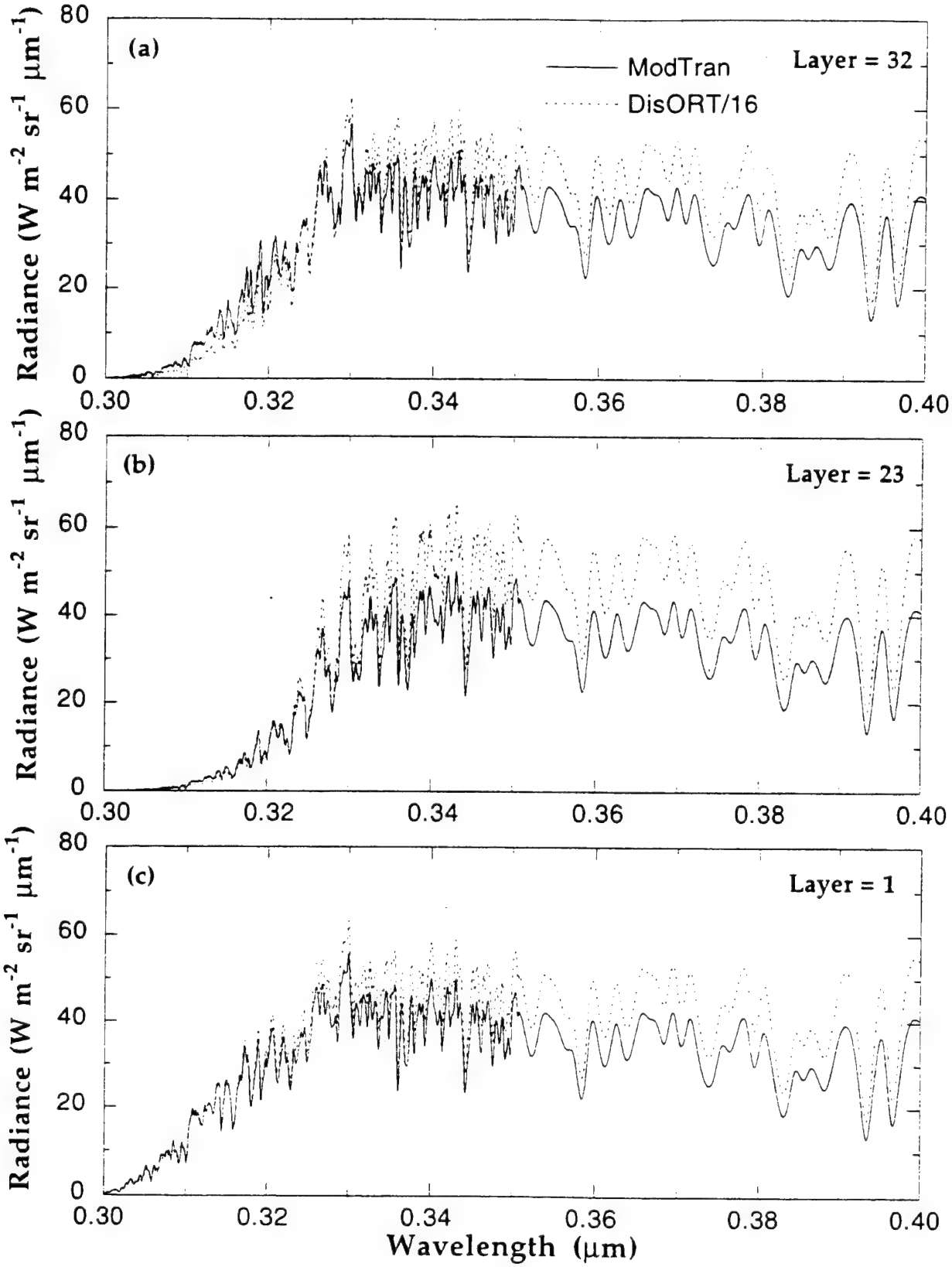

Figure 1. Source function computed from MODTRAN and DISORT with 16-stream at the (a) top, (b) middle and (c) bottom for a clear subarctic winter atmosphere (see text for details).

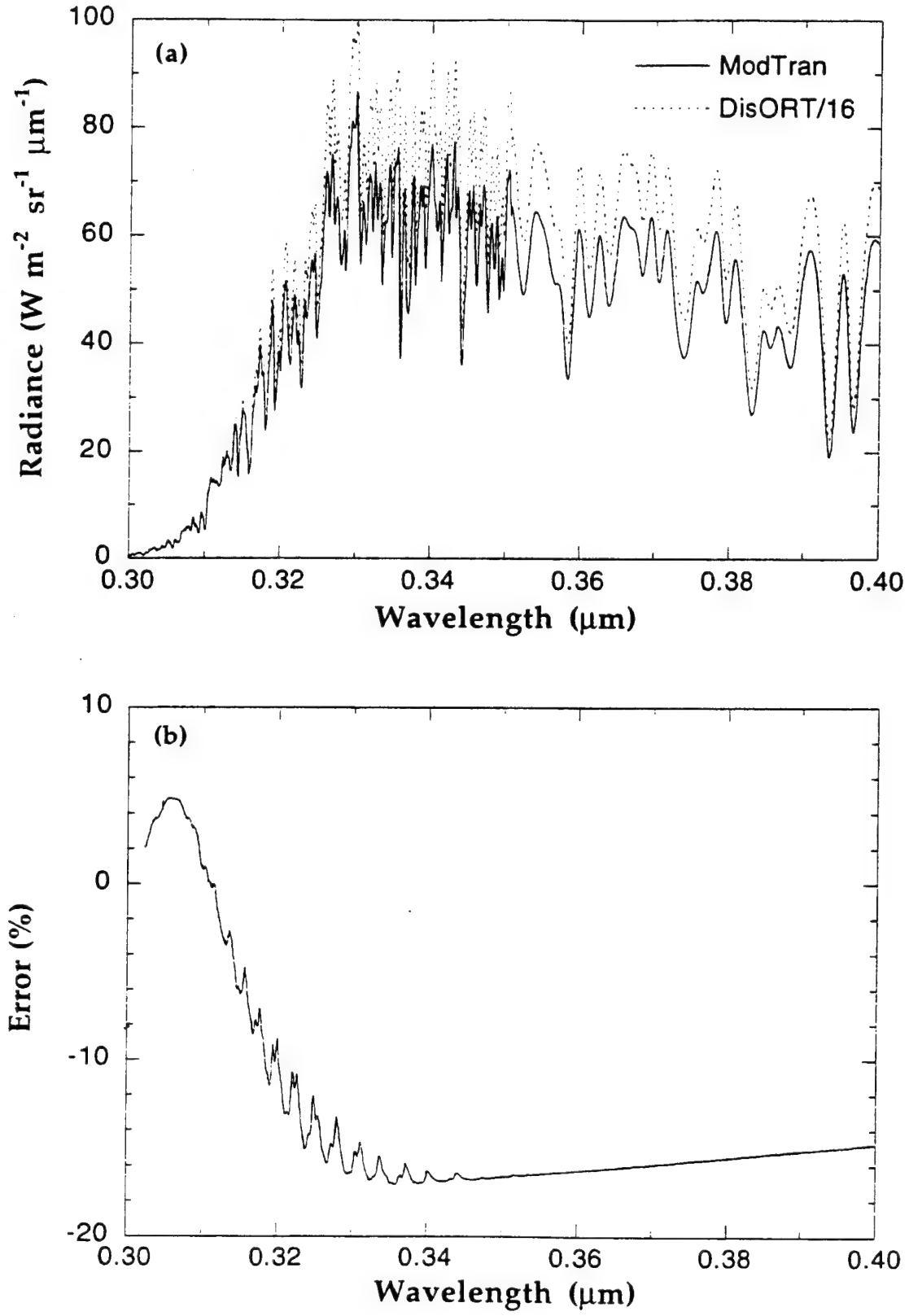

Figure 2. Same as in Figure 1, but for (a) total radiance and (b) error (see text for details).

Finally, we should mention an existing problem with MODTRAN (of which the Air Force staff are already aware): the single scattering albedo occasionally exceeds one (a physically impossible value). This problem can be "fixed" by an "if test" setting the single scattering albedo identically to one whenever it exceeds one. Such a "fix" should be considered as temporary, however, since it may not completely resolve problems connected with this "anomaly" in the code. Thus, there is a need to address this problem.

4.2. DISORT/FASCODE Merging and Validation

From a physical point of view, the main difference between MODTRAN and FASCODE lies in the treatment of molecular spectroscopy and frequency sampling. Whereas MODTRAN is a sophisticated narrow-band model which employs "fixed frequency" steps at 1 cm^{-1}, FASCODE is a line-by-line code which uses different frequency step size at each atmospheric layer, depending on local temperature, pressure, and line width. The merging of DISORT and FASCODE is made difficult by this spectral sampling strategy adopted in FASCODE to optimize its computational efficiency, because DISORT requires "fixed frequency" steps. This sampling strategy is a unique feature of FASCODE, which is not employed in other line-by-line codes such as GENLN2 (Edwards 1992).

To get started on the merging of DISORT with FASCODE it was decided to make FASCODE compatible with DISORT by using an interpolation scheme to interpolate optical depths to "fixed frequency" steps. As already mentioned, this procedure has the advantage that it would also provide a framework within which "benchmark" line-by-line multiple scattering computations could be accomplished by combining FASCODE and DISORT. Such benchmarks are necessary for testing purposes in the development of a merged FASCODE/DISORT code with rigorous multiple scattering and optimum frequency sampling.

The first step in the merging consisted of the computation of gaseous optical depth from FASCODE at "fixed frequency" steps by interpolating between layers. The four-point Lagrangian interpolation scheme that is already used in FASCODE to interpolate absorptances proved (not surprisingly) to be adequate for this purpose. This approach allowed us to obtain optical depth at all layers in the atmosphere at

fixed wavenumbers. For testing purposes, we have chosen a clear US standard atmosphere (Anderson et al., 1986) as the background profile. The surface temperature was set at 294.2 K and the viewing direction corresponds to an observer located at 10 km height (10 layers below with 1 km thick each) looking downward at nadir. To check that these optical depths were correct we used the GENLN2 (Edwards, 1992) code to compute optical depth at the same fixed wavenumber intervals. Care was exercised to make sure that the input to the two codes was identical. Comparisons (e.g., at 6.3 μm water vapor and 15 μm carbon dioxide absorption bands) showed that the two codes gave almost identical "fixed frequency" optical depths. Corresponding tansmittance and radiance fields computed by the two codes were also identical. The next step consisted of feeding the optical depths from FASCODE into DISORT to compute radiances off-line.

Having tested that the radiances returned from DISORT were the same as those computed by FASCODE, we finally merged the two codes so that DISORT was called directly from FASCODE. The previous two examples obtained by the original FASCODE and FASCODE merged with DISORT are shown in Figures 3 and 4. The results shown in Figure 3 were for the spectral region 6.3 μm with water vapor as the only active gas. The merged FASCODE/DISORT package produced slightly higher radiance values but within about 0.4%. Similar comparisons between original FASCODE and the merged FASCODE/DISORT package for the 15 μm carbon dioxide absorption band were also shown in Figure 4. Good agreements were obtained for this region. More thorough tests across the entire spectrum are needed to confirm the validity of this merging between the FASCODE and DISORT codes.

5. Discussion

It may eventually be desirable to include full azimuth-dependence in MODTRAN. This will require a major effort because MODTRAN needs to be modified significantly to accomplish this. We think this would be feasible, however, by using MODTRAN to calculate optical properties and geometry effects and using DISORT to do the complete radiative transfer computation including single and multiple scattering.

The advantage of the current implementation of DISORT into MODTRAN is that it requires only minor changes to the existing MODTRAN structure. The disadvantage is that the current implementation does not allow us to take full

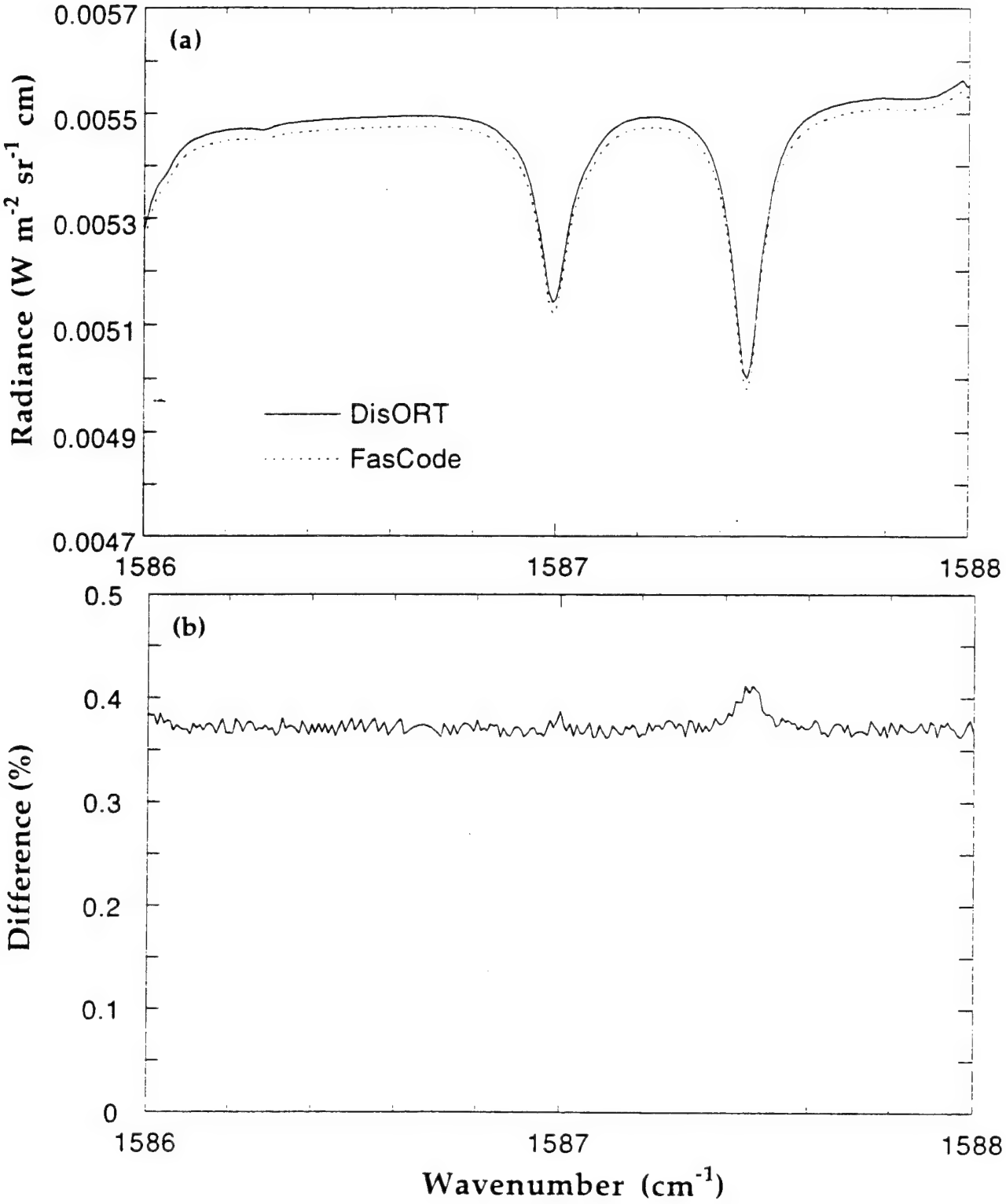

Figure 3. Comparisons between the original FASCODE and the merged FASCODE/ DISORT package at 6.3 μm water vapor absorption band for (a) radiance and (b) difference for a clear US standard atmosphere (see text for details).

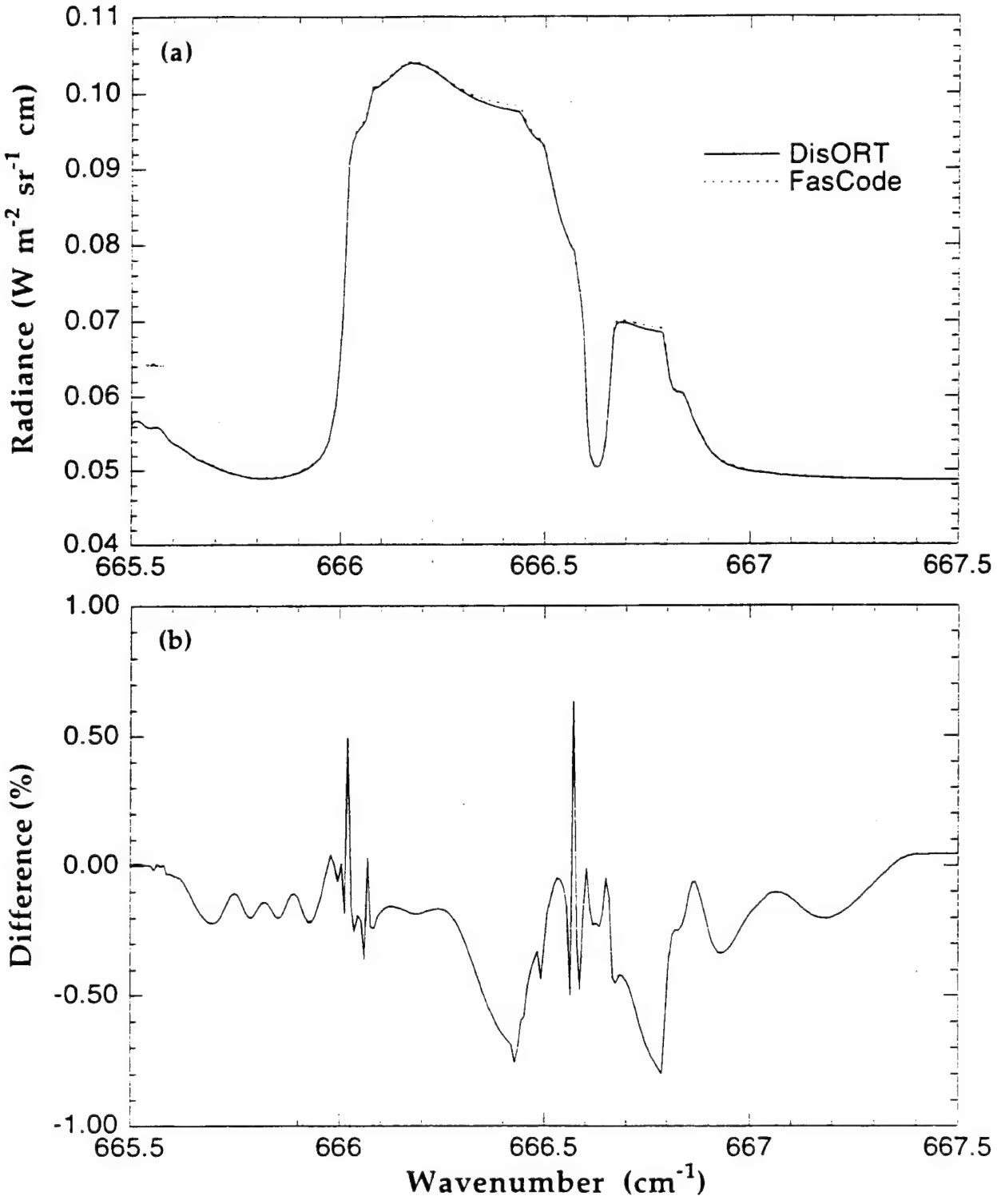

Figure 4. Same as in Figure 3, but for 15 μm carbon dioxide absorption band (see text for details).

advantage of the DISORT code which has several attractive features including the computation of the full azimuth dependence of the intensity. It also guarantees that the computation of the source function and the intensity are done consistently. For example, the current version of DISORT uses a linear-in-optical-depth dependence of the Planck function. Whereas the original version of MODTRAN used a cruder approximation (assuming the Planck function to be constant within each layer) to integrate along the line-of-sight to obtain the intensity from the source function, this limitation in MODTRAN has been removed by the implementation of a linear-in-optical depth dependence. There are basically two ways in which to proceed: (i) the complete radiative transfer computation including thermal and direct beam contributions is handled by DISORT, or else (ii) the current version of MODTRAN is used which allows a linear-in-optical depth dependence of the Planck function within each atmospheric layer. The second option would provide a consistent treatment of thermal radiation in MODTRAN and DISORT and would probably be the easiest to implement. Also it would not require significant changes in current MODTRAN structure.

Nevertheless, we strongly recommend that the first option eventually be implemented in MODTRAN to take full advantage of the superior capabilities of the DISORT code with respect to solving the radiative transfer problem including multiple scattering and surface bidirectional reflectance. We should also point out that a new version of DISORT will soon be released in which the speed of the intensity computation will be substantially improved, and in which an exponential-linear-in-optical depth dependence of the Planck function will be used to obtain accurate solutions for atmospheric layers with steep temperature gradients. The exponential-linear-in-optical depth approximation is much superior to the linear approximation for optically-thick situations (Kylling and Stamnes, 1992). These improvements in the new version of DISORT makes it even more desirable to use MODTRAN to calculate optical properties and geometry effects, but employ DISORT to do the complete radiative transfer computation including single and multiple scattering. This approach would also guarantee that the computation of the source function and the intensity are done consistently. As already mentioned, the new version of DISORT uses an exponential-linear-in-optical depth dependence of the source function, whereas the current version of MODTRAN assumes a linear

dependence of the Planck function to integrate along the line-of-sight to obtain the intensity from the source function. Thus, even though the MS contribution to the source function is computed very accurately by using DISORT (which applies the exponential-linear approximation), some of this accuracy may be lost unless its integration along the line-of-sight is improved.

An important step in the merging of DISORT into FASCODE has been accomplished by combining DISORT and FASCODE in a "fixed frequency" mode. This has allowed us to establish a testbed for "benchmark" computations against which we may explore and test future computational schemes including optimum frequency sampling strategies designed to maximize efficiency. One possible way to proceed in the pursuit of an efficient yet accurate inclusion of multiple scattering in line-by-line codes is to exploit spectral mapping transform techniques. In essence this approach consists of reducing the need for multiple scattering computations by exploiting the existing redundancy in absorption coefficients across a given spectral interval over which the scattering coefficients do not vary appreciably. Such an approach will require some disk space, but this is not considered a serious limitation since disk space is relatively inexpensive nowadays.

6. Summary

A state-of-the-art radiative transfer algorithm (DISORT) has been interfaced with MODTRAN to provide a rigorous treatment of multiple scattering effects. This "marriage" between DISORT and MODTRAN includes the development of new compatible routines with suitable interfaces as required to "consumate" the marriage.

Currently MODTRAN is seeking only the azimuthally-averaged component (i.e., the zero-order Fourier component of the intensity) of the multiply-scattered intensity (from DISORT or BMFLUX). The single scattering contribution is computed in MODTRAN and combined with the multiple scattering part from DISORT (or BMFLUX) and integrated along the line-of-sight to yield the intensity in the desired direction. In the thermal infrared part of the spectrum this is the complete intensity because there is no azimuth dependence. In the solar part of the spectrum this approach ignores the contribution of multiple scattering to the first and higher-order Fourier components of the intensity. When multiple scattering is important there will be an error in the azimuthal dependence of the intensity

predicted by the present interfacing of DISORT and MODTRAN. This error is expected to be negligible for thermal cases where the solar contribution is small, but may be significant in spectral regions where solar radiation dominates depending on atmospheric conditions, solar zenith angle and viewing geometry. It is possible to avoid such errors by using MODTRAN to compute optical properties and geometry effects, but employing DISORT to do the complete radiative transfer computation including all orders of multiple scattering. It would be desirable to upgrade MODTRAN to include this capability in the future.

Finally, we note that since DISORT efficiently computes fluxes and mean intensities, it would be relatively easy to add the capability of computing fluxes and warming/cooling rates and photolysis rates in MODTRAN. We expect warming and cooling rates computed from MODTRAN and DISORT to be quite accurate throughout the troposphere and stratosphere for spectral regions where the narrow-band model approch underlying MODTRAN provides an adequate 'quasi-monochromatic' description of the radiaitve transfer. Preliminary tests show that whereas the merged package yields reliable warming rates for solar wavelenghts, such is not the case in the thermal infrared. Here the current band model must be combined with a suitable "k-distribution". Once a reliable "k-distribution" has been implemented into a future version of MODTRAN (and properly tested), we expect a merged version of MODTRAN and DISORT to be capable of providing accurate ("benchmark") results for development of parametrized treatments of warming/cooling rates. Currently, more costly line-by-line computations are used for this purpose. Thus, we would like to emphasize that the merged package could be extended to offer several enhanced capabilities over the original MODTRAN code:

- through the use of DISORT several additional quantities are available in the merged package (as compared to the original MODTRAN) such as
  - (i) net flux and its divergence;
  - (ii) direct-beam flux, diffuse upward and downward fluxes;
  - (iii) mean intensity (or actinic flux), and azimuthally-averaged intensity;
  - (iv) the angular intensity including full azimuthal dependence;
- intensities may be computed at arbitrary angles;
- intensities and fluxes may be computed at arbitrary levels.

Therefore, the merged code is expected to become a most valuable research tool in remote sensing and atmospheric science applications. For example, the computation of the mean intensity by DISORT allows for accurate computations of atmospheric photolysis and warming/cooling rates which play an important role in atmospheric dynamics and chemistry as well as in climate applications. It will also provide a reliable tool for the computation of biologically relevant ultraviolet radiation and the potential impact of ozone depletion on ultraviolet radiation exposure.

A merged version of DISORT and FASCODE has been accomplished in a "fixed frequency" mode in which the gaseous optical depths computed in FASCODE are interpolated to the same frequency step size in all atmospheric layers. In contrast to the existing multiple scattering scheme in FASCODE (Isaacs et al., 1986) this merged package is computationally slower because it cannot take advantage of the spectral sampling strategy which allows the existing implementation based on the adding-approach to reduce the number of multiple scattering computations in a vertically inhomogeneous medium. On the other hand, the adding-approach results in a factor of 3 increase in CPU time and storage requirements due to the required merging of stored quantities, which is entirely avoided in the merging of FASCODE with DISORT in the "fixed frequency" mode. Instead this time can be spent on accurate multiple scattering computations. With respect to efficiency we note that the computational speed for a particular run of the original FASCODE as compared with the merged FASCODE/DISORT package, must be viewed in light of the amount of information each code produces. Whereas FASCODE has to be executed over and over again for each atmospheric path and each new viewing direction, the merged FASCODE/DISORT package yields information at all desired locations and viewing directions in a single run at insignificant additional cost.

Thus, if output at say 10 viewing angles and 10 atmospheric levels is desired, the original FASCODE would have to executed 100 times as compared to a single run of the merged package. For such an application we conjecture that the merged package would provide accurate results at a very "competitive price." It is important to note that the merging of FASCODE and DISORT provides a testbed for "benchmark" computations including multiple scattering against which alternative approaches aimed at enhanced efficiency may be tested. A spectral mapping procedure is identified as a potential candidate for future attempts to optimize the merged FASCODE/DISORT package with respect to computational speed.

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Appendix: Further Validation of DISORT/MODTRAN Merging

a. Further Comparisons in the solar spectral region

Comparisons of MS source function profiles at 350 nm are shown in Figure A1 for clear and hazy sky conditions. As shown in Figure A1a, the vertical source function profiles calculated by MODTRAN are roughly under-estimated by about 50% for clear sky. With the introduction of aerosols (IHAZE=2, boundary-layer rural-aerosol model of 5 km visibility range), the absolute magnitude of source function increases as expected, but remains underestimated by about 50%. Figure A1b depicts the relative errors, ranging from -12% to -35% with a peak near the tropopause for clear sky and near the boundary layer for hazy sky conditions. These errors are expected and can be corrected since the computations of source function between the MODTRAN and DISORT have several differences, as discussed in detail in Section 4.1.

A similar comparison of multiple scattering source functions and total spectral radiances for the visible region between 0.58 and 0.60 μm is shown in Figure A2 for a clear subarctic atmosphere illuminated by the sun at a zenith angle of 60° with an observer looking straight down. The MODTRAN and the merged version with DISORT 2-stream results are similar, and they both underestimate the total radiance by less than 10% as compared to the accurate DISORT 16-stream results. A comparison of MS source function profiles for this case is shown in Figure A2b at 0.60 μm. The differences between the MS source functions obtained using MODTRAN and the merged package can become as large as 100% in the lower troposphere. Hazy cases (IHAZE=1 and 2) also show similar behavior (figures not shown).

b. Comparisons in the solar and thermal crossover region

Next we look at the crossover region where both solar and thermal radiation contribute. The subarctic winter atmosphere with hazy (IHAZE=2) conditions was chosen here for investigation in the 3.5 to 4.0 μm region. The solar zenith angle is 60° and an observer is located at 100 km height looking straight down. The spectral radiance escaping from the top of the atmosphere in the zenith direction is shown in Figure A3 for the total, solar and thermal components. There is good agreement between results obtained by MODTRAN and by the merged package with varying

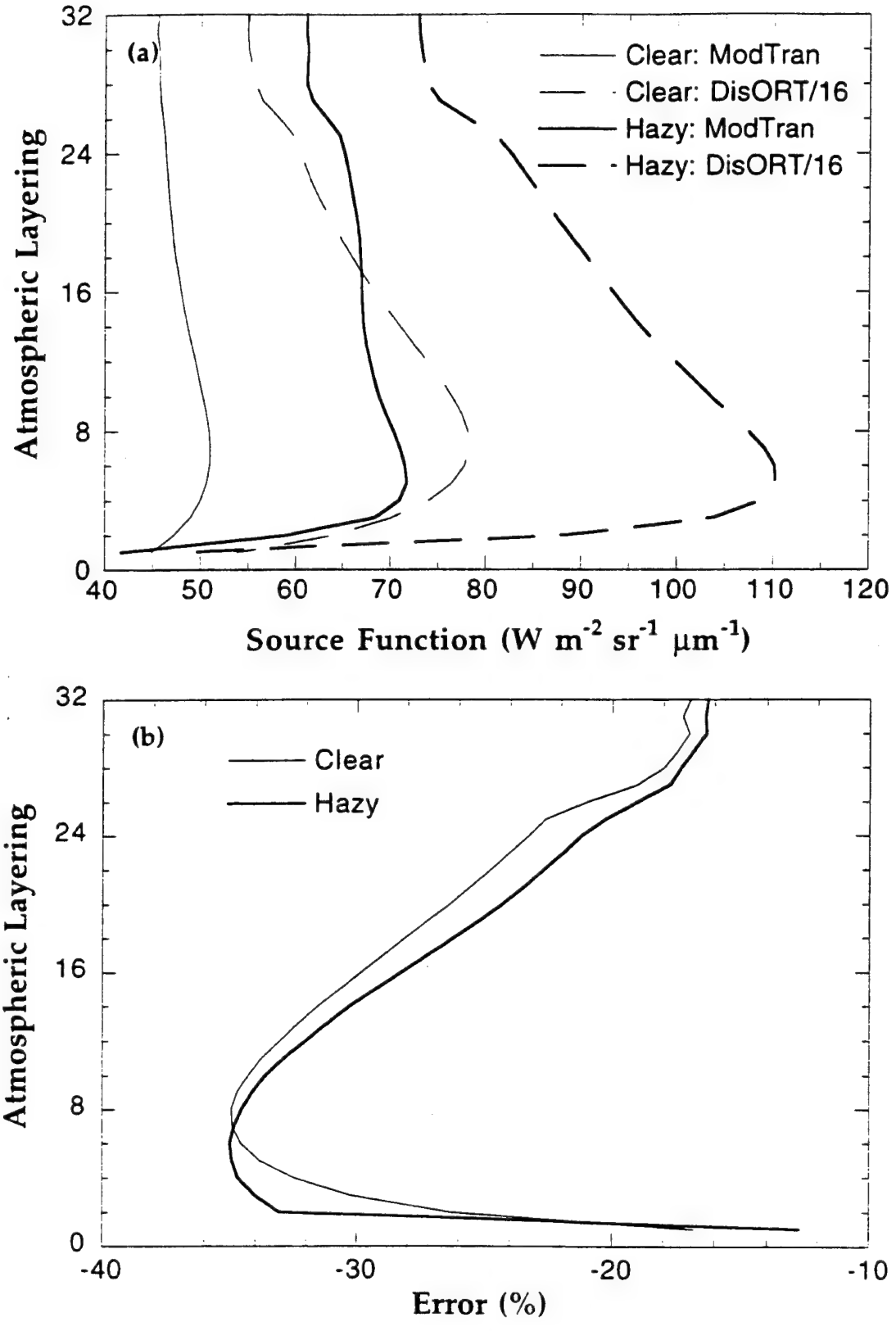

Figure A1. Vertical profiles of subarctic winter atmosphere with hazy conditions at wavelength of 350 nm for (a) source functions and (b) errors (see text for details).

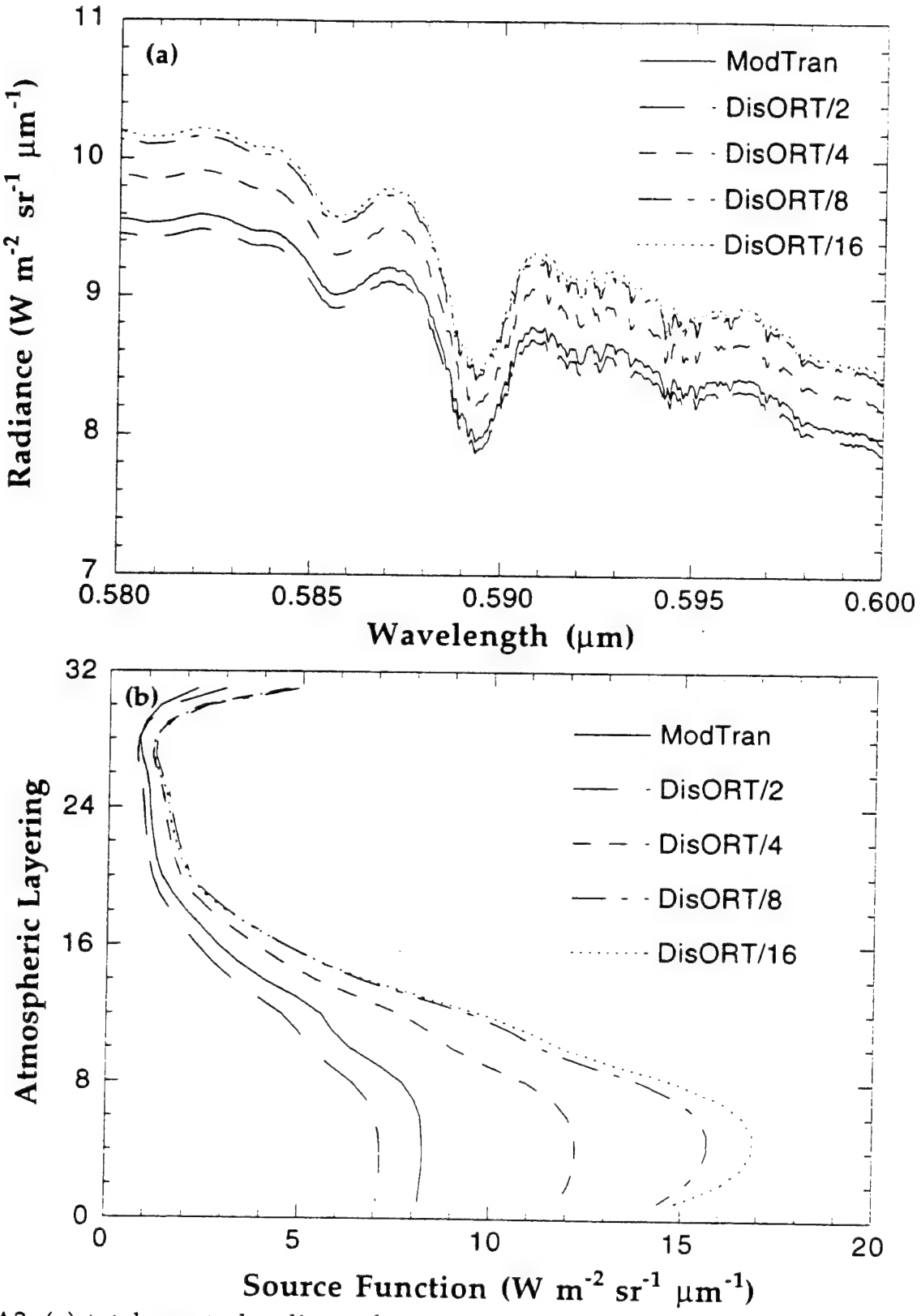

Figure A2. (a) total spectral radiance from 0.58 to 0.60 μm and (b) source function profiles at 0.6 μm computed from MODTRAN and DISORT with varying number of streams for a clear subarctic winter atmosphere (see text for details).

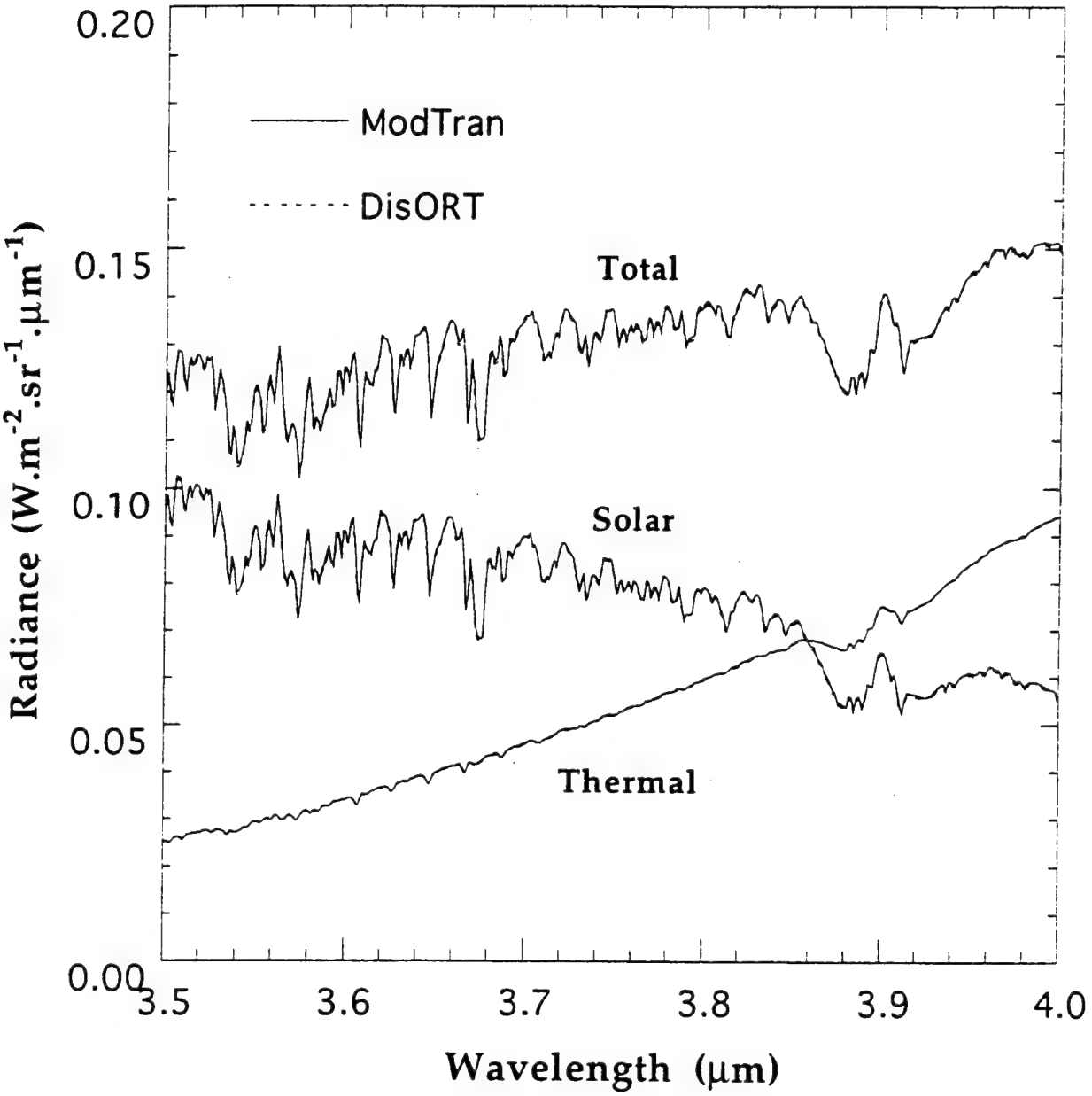

Figure A3. Total, solar and thermal spectral radiance from 3.5 to 4.0 μm computed from MODTRAN and DISORT with varying number of streams for a hazy subarctic winter atmosphere (see text for details).

number of streams in DISORT. This is also expected by looking at Figure A4, which shows MS source function profiles at 3.86 μm where the solar (top panel) and thermal (bottom panel) components are of similar magnitude. The solar and thermal MS source functions at different atmospheric layers also show similar behavior in the entire 3.5 to 4.0 μm region.

c. Comparisons in the thermal spectral region

Multiple scattering source functions in the thermal region between 5 and 25 μm are displayed in Figure A5 for a clear subarctic winter atmosphere, and in Figure A6 for a hazy (IHAZE=2) situation. We note the excellent agreement between the computed source functions in the middle of the atmosphere (e.g., layer 23) for both cases, whereas there is some disagreement in the top layer, which may be due to different treatments of the temperature variation between MODTRAN2 and DISORT. In MODTRAN2, the thermal source is computed assuming that the atmospheric layers are isothermal, whereas in DISORT the Planck function is computed from the actual temperature assigned to the top and bottom of each layer and then assumed to vary linearly with optical depth across each layer. In the bottom layer the source functions are the same for the clear sky situation, but there is noticeable difference in two regions (8-14 μm, 17-21 μm) for the hazy situation. Between 8 and 14 μm there is also some dependence on the number of streams used in the DISORT computation indicating the relatively strong contribution from scattering in this spectral range.

The total spectral radiance corresponding to Figures A5 and A6 are shown in Figures A7 and A8 for the clear and hazy sky situation, respectively. The upper panels show the downward (nadir) radiance at the surface. The plots for the clear and hazy condition look very similar except for discernible differences in the 8-14 μm region as expected due to the haze. Note, however, that there is little difference between MODTRAN2 results and those produced using DISORT, indicating the relatively small contribution from multiple scattering to the total spectral radiance even in the hazy situation. The lower panels show the upwelling radiance escaping form the top of the atmosphere in the zenith direction. There is no discernible difference between the clear and the hazy situation, nor between the MODTRAN2 results and those produced using DISORT, which is expected because the radiance emerging from the top of the atmosphere would be insensitive to the aerosol loading in the troposphere.

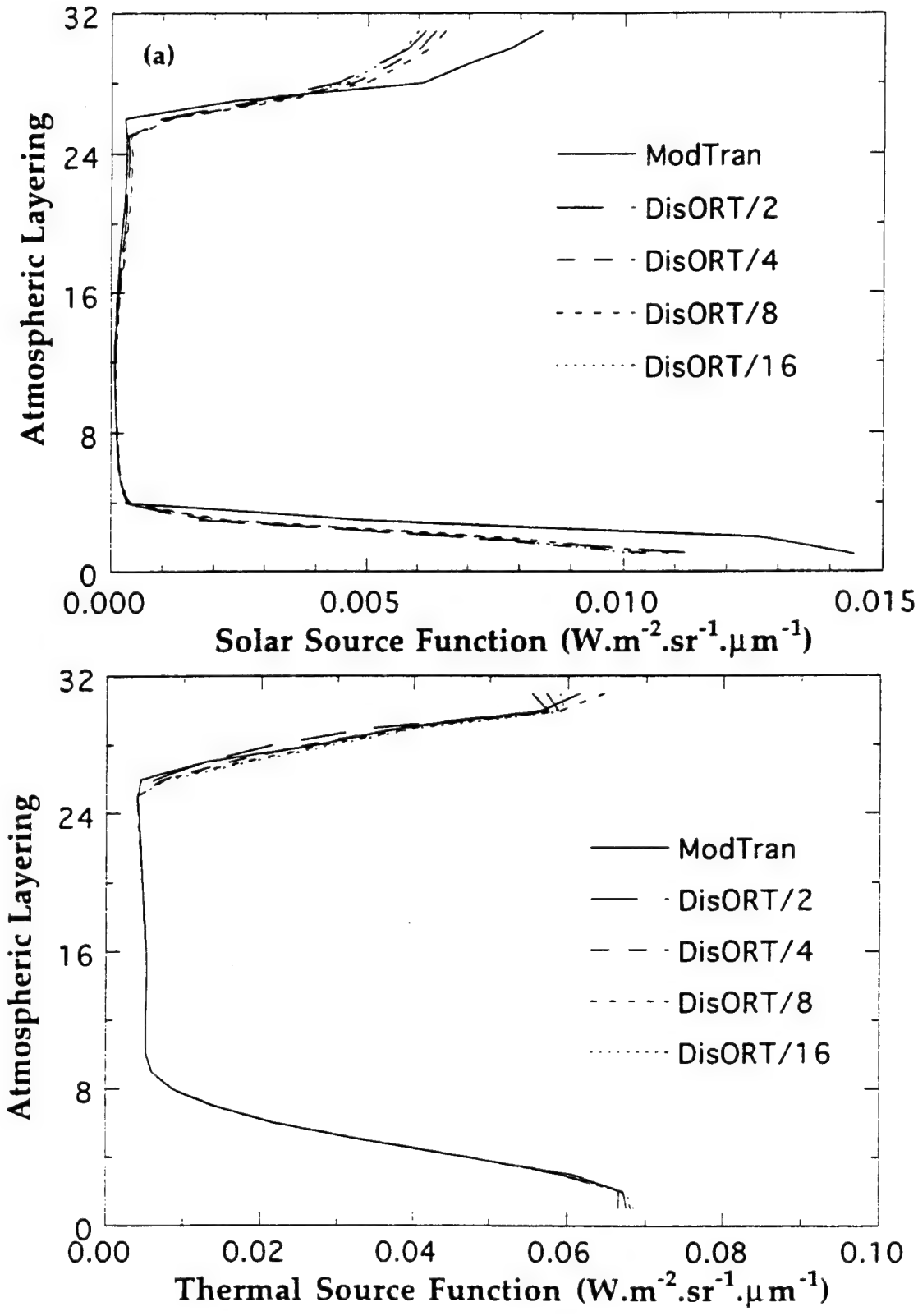

Figure A4. Same as in Figure A3, but for vertical profiles at wavelength of 3.86 μm for (a) solar and (b) thermal source functions (see text for details).

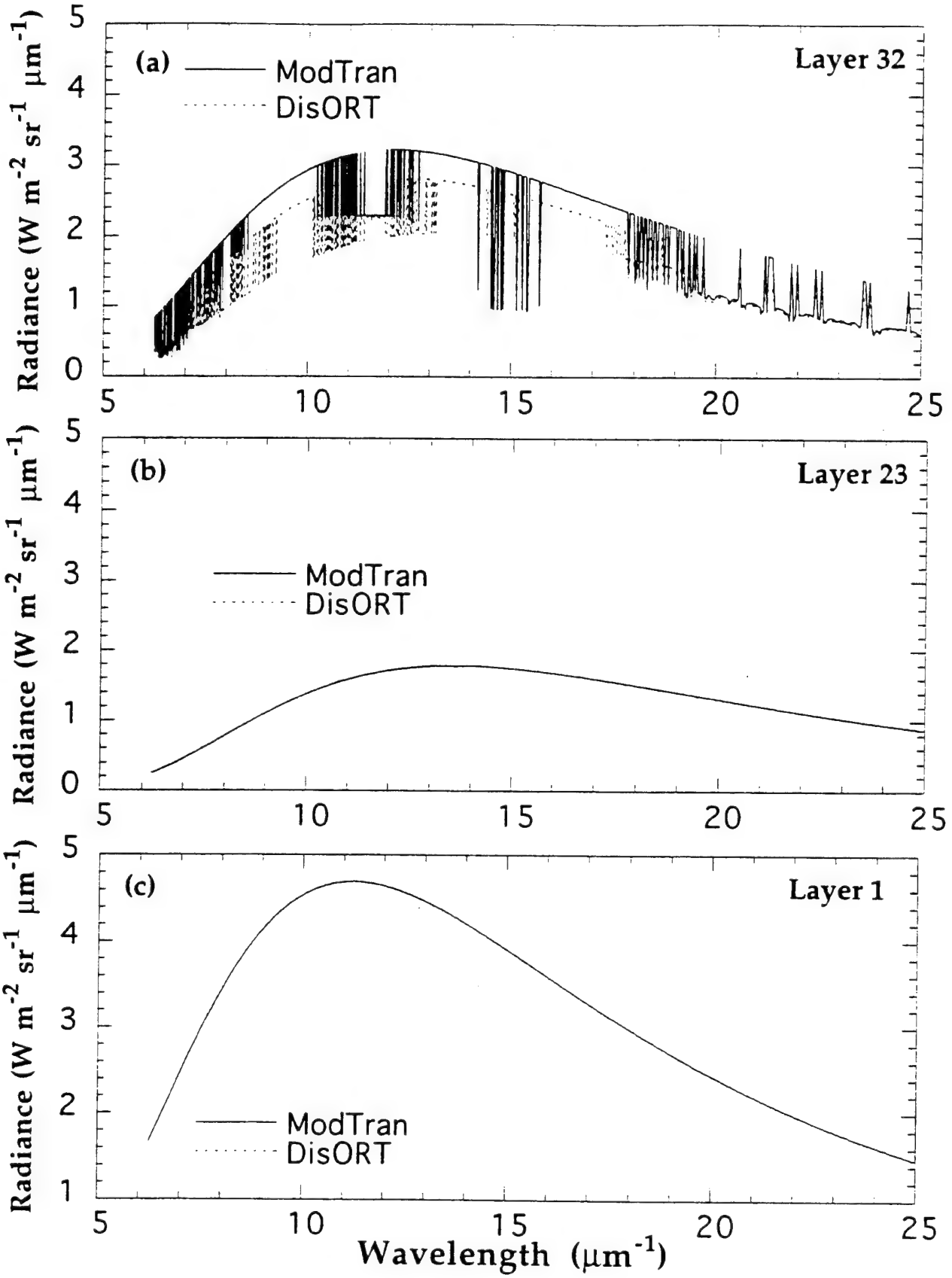

Figure A5. Source function computed from MODTRAN and DISORT with varying number of streams at the (a) top, (b) middle and (c) bottom for a clear subarctic winter atmosphere (see text for details).

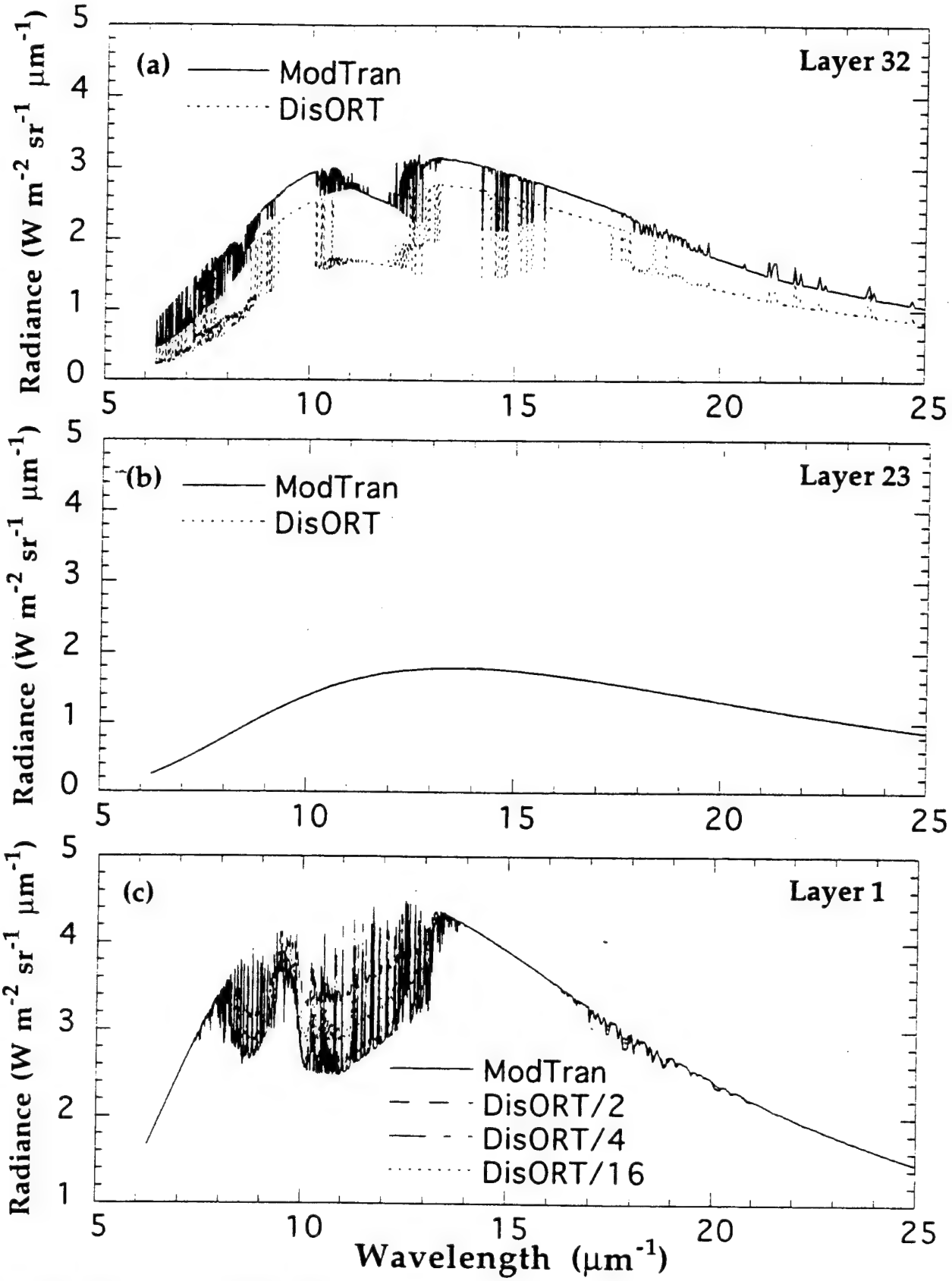

Figure A6. Same as in Figure A5, but for a hazy subarctic winter atmosphere (see text for details).

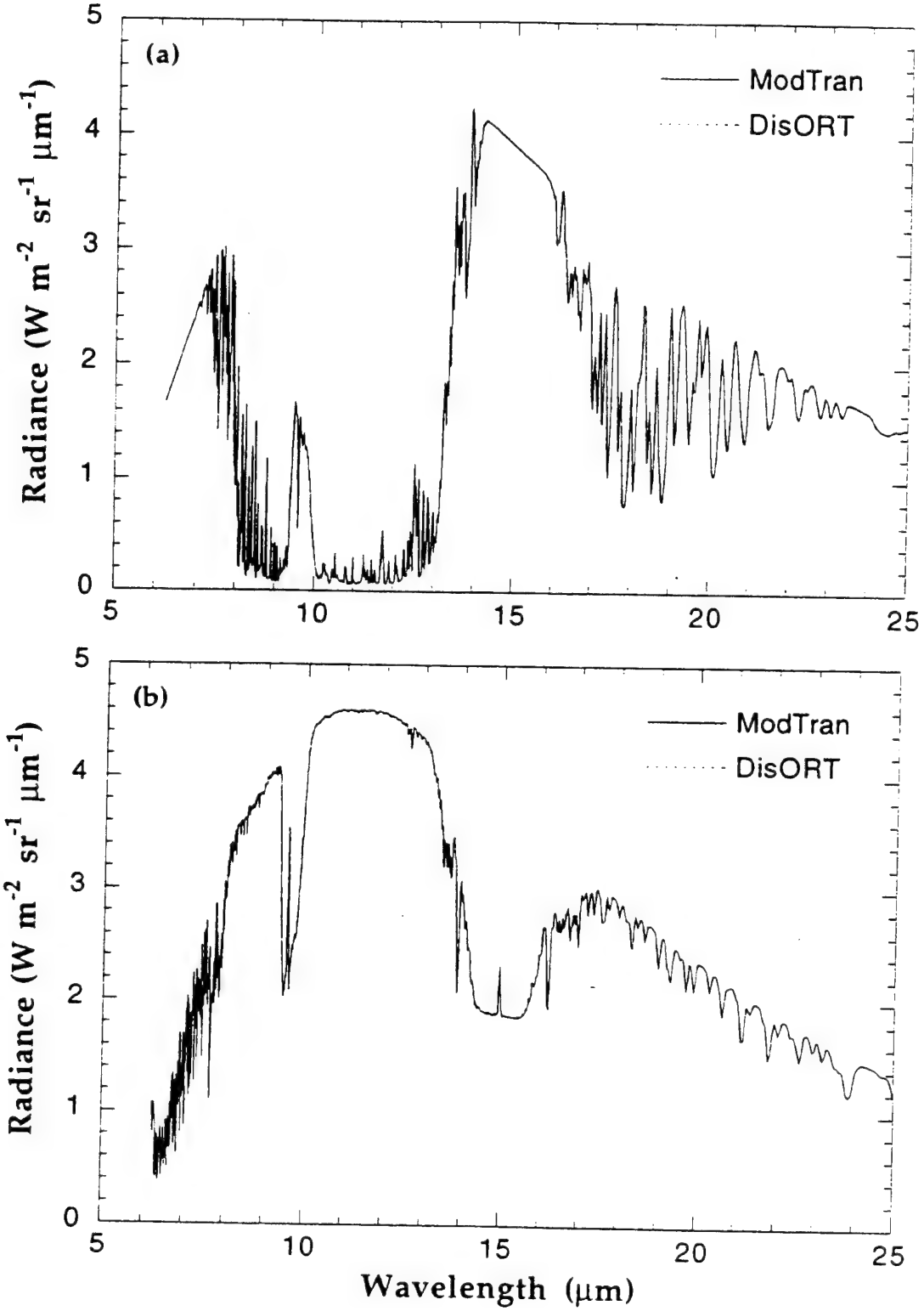

Figure A7. Total spectral radiance computed from MODTRAN and DISORT with varying number of streams at the (a) surface (nadir) and (b) top (zenith) for a clear subarctic winter atmosphere (see text for details).

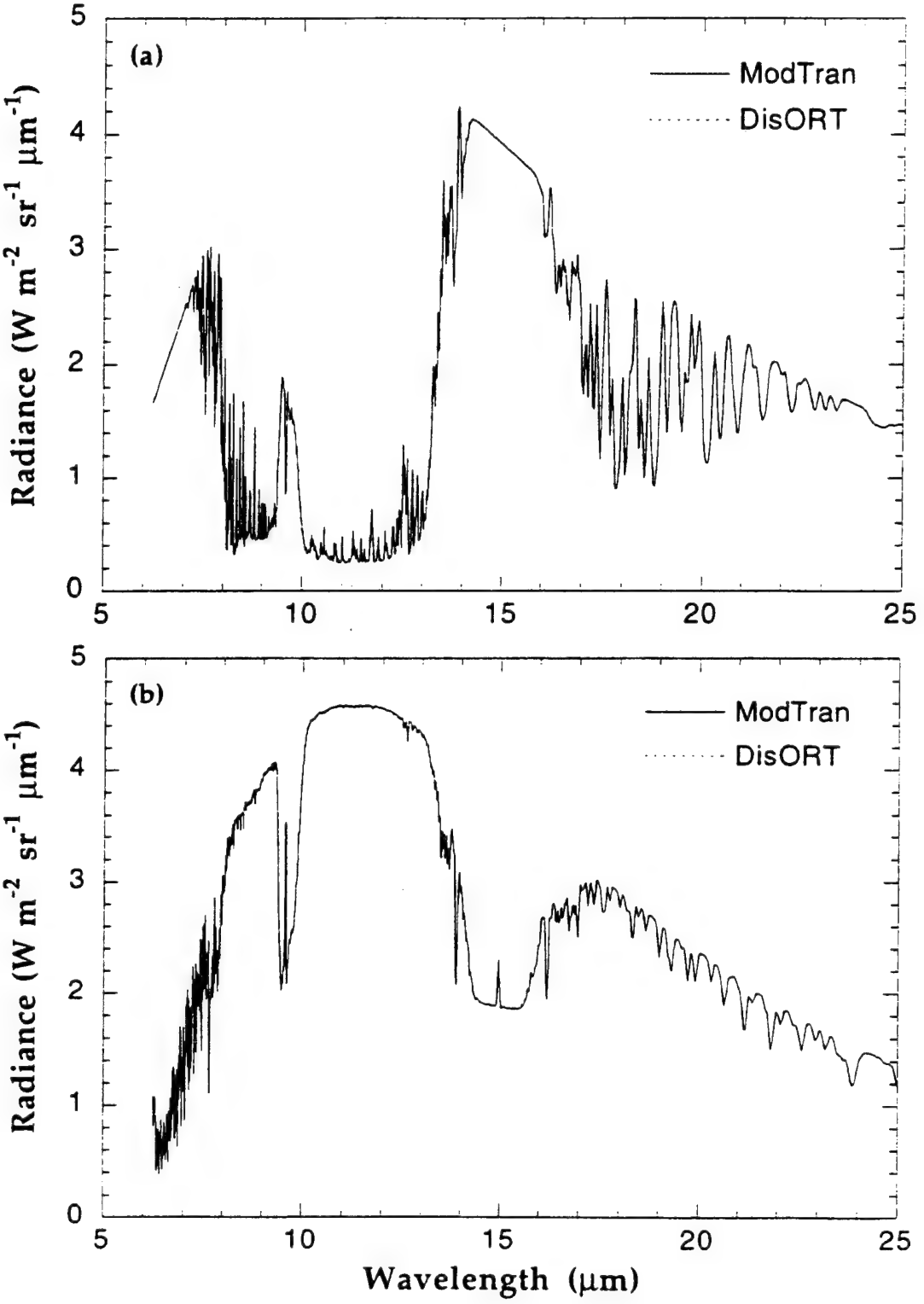

Figure A8. Same as in Figure A7, but for a hazy subarctic winter atmosphere (see text for details).

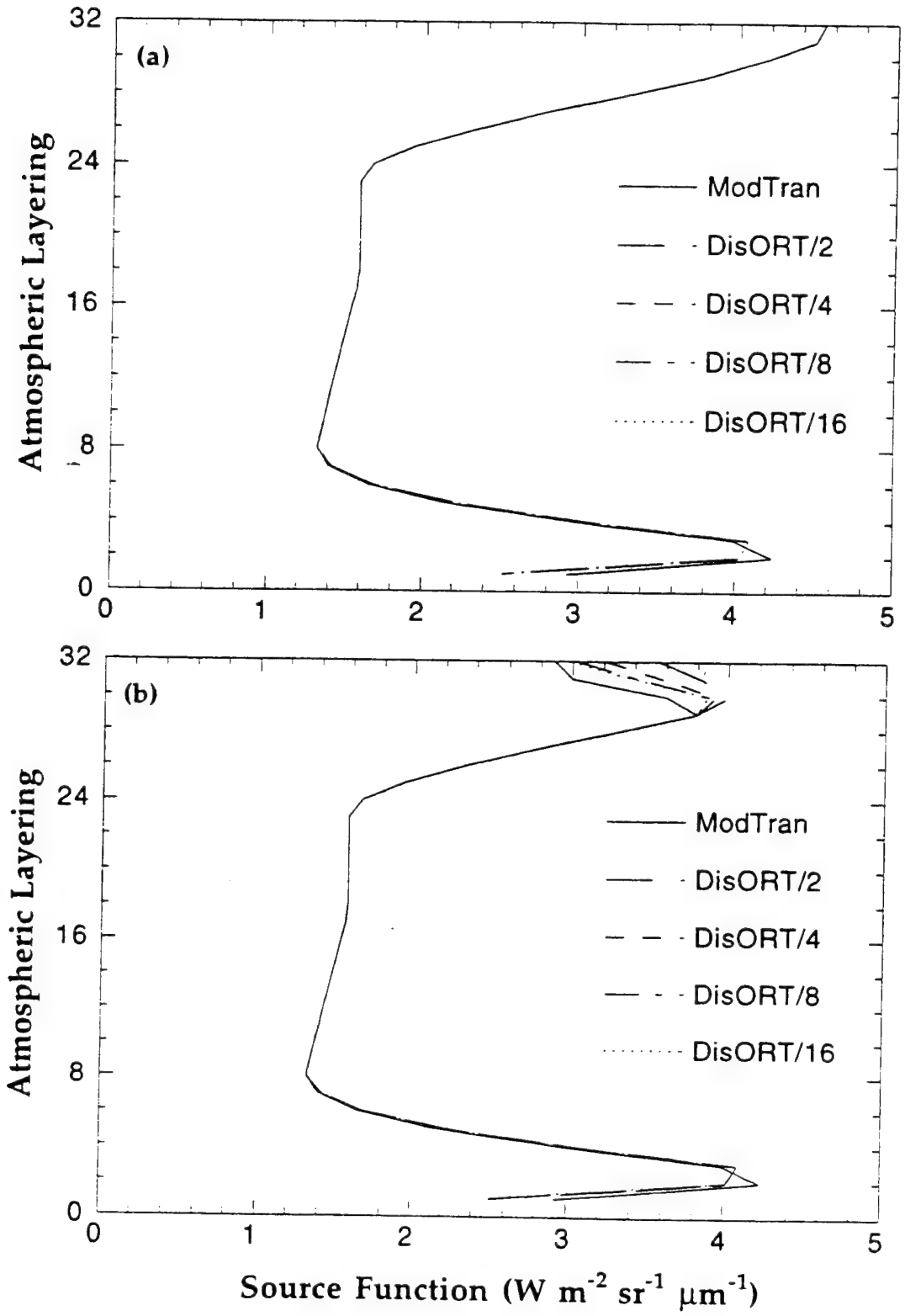

Figure A9. Source function profiles computed from MODTRAN and DISORT with varying number of streams at 10 μm for a (a) clear and (b) hazy subarctic winter atmosphere (see text for details).

Finally, vertical profiles of the thermal MS source functions at 10 μm computed from MODTRAN2 and the merged package of DISORT with varying number of streams are shown in Figure A9 for clear as well as hazy sky conditions. Overall, the structure of the computed MS source functions for both cases is quite similar throughout the entire atmosphere.

d. Comparisons with experimental data from the SPECTRE campaign

As a final example we discuss briefly some comparisons with experimental data obtained during the SPECTRE (SPECTral Radiance Experiment) campaign conducted at Coffeyville, Kansas in December 1991. In 1988, the International Radiation Commission (IRC) and the World Climate Research Program (WCRP) both endorsed a program to validate the ability of the many radiation schemes used in climate models by comparing results with observations. The SPECTRE was the outgrowth of this joint endorsement.

During the SPECTRE, observations of vertically downwelling radiance in the 520 to 3020 cm^{-1} region were obtained using FTIR (Fourier Transfer Infra-Red) spectrometers with spectral resolution ranging from 0.1 to 2 cm^{-1}. Profiles of temperature, water vapor, and ozone were obtained concurrently using radiosonde, Raman lidar, and RASS (Radar Acoustic Sounding System). The data were obtained during clear sky conditions on four different days, during which the meteorological conditions were in transition from midlatitude summer to midlatitude winter. The data were taken by the University of Wisconsin's Atmospheric Emitted Radiance Interferometer (AERI) instrument, which has advanced data quality control (R. Ellingson, personal communication, 1993). The AERI is a zenith-viewing instrument possessing a spectral resolution of 0.5 cm^{-1}, covering two spectral regions, 520-1800 cm^{-1} and 1800-3020 cm^{-1}.

The computations used the best resolution available in the model, 1 cm^{-1}, which is twice the resolution of the AERI instrument. Profiles of pressure, temperature, water vapor, and ozone were provided at 45 atmospheric levels along with the measured spectra. Since MODTRAN2 allows a maximum of only 34 levels, the measured profiles were interpolated among the higher levels below 30 km to provide profiles suitable for use in MODTRAN2. The interpolated profiles are shown in Figure A10, and profiles above 30 km are adopted from a clear mid-latitude winter atmosphere (Anderson et al., 1986). The measured spectra were

modeled in two different ways: (i) using the original MODTRAN2, (ii) using the merged MODTRAN2/DISORT package. A third approach using MODTRAN2 to compute the optical properties and DISORT with 16 streams to do the complete radiative transfer computation gave results identical to the merged package. Comparisons of the measurements and the computed spectra are shown in Figure A11 for the 500-2000 cm^{-1} spectral range, and in Figure A12 for the 2000-3000 cm^{-1} spectral range. Note that MODTRAN2 alone and the merged package yields almost identical results as they should in the absence of significant multiple scattering contributions to the radiation field. Finally, the difference between the MODTRAN2 and the merged package is displayed in Figure A13.

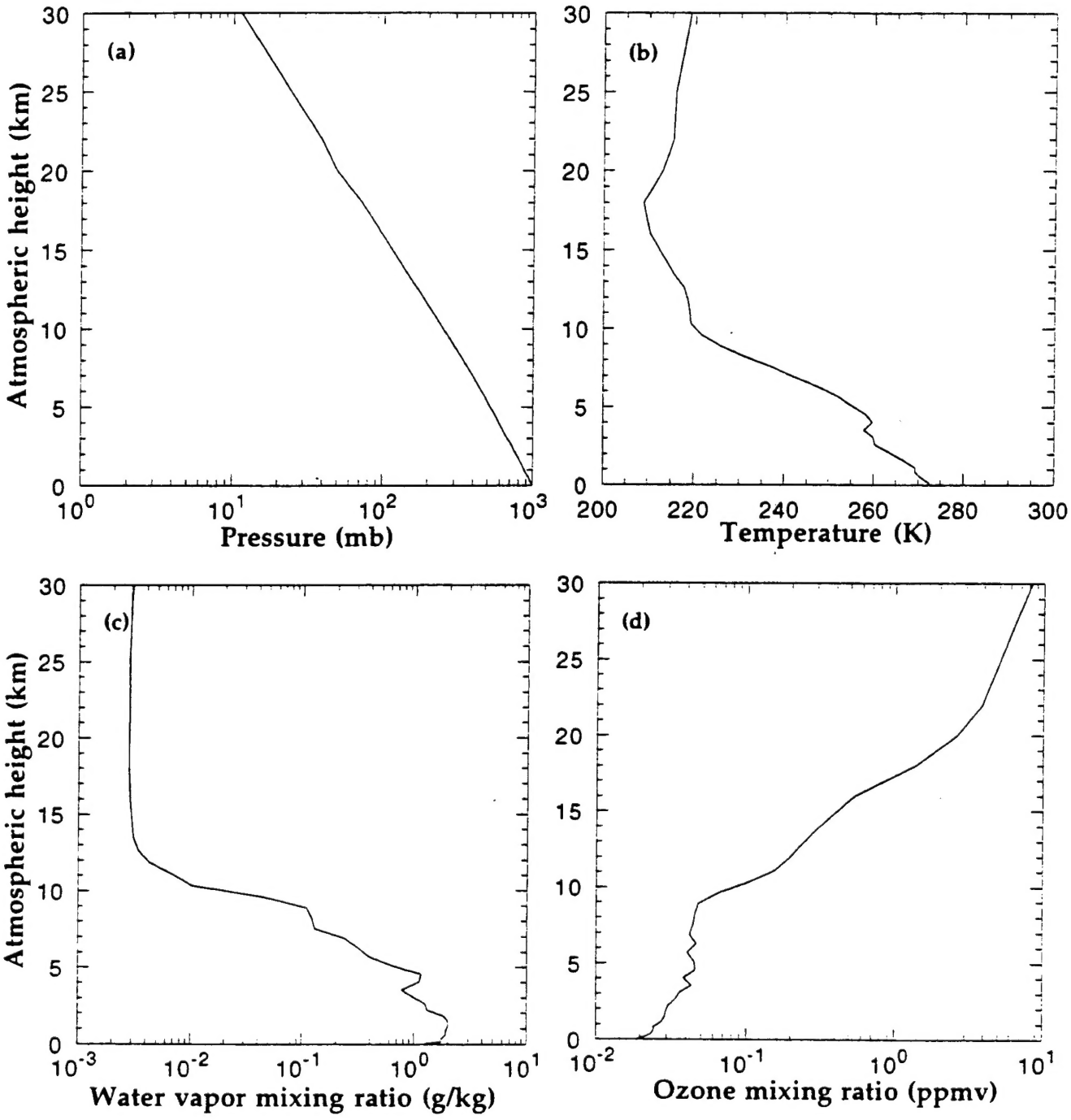

Figure A10. Interpolated atmospheric profiles of (a) pressure, (b) temperature, (c) water vapor mixing ratio, and (d) ozone mixing ratio for modeling calculations (see text for details).

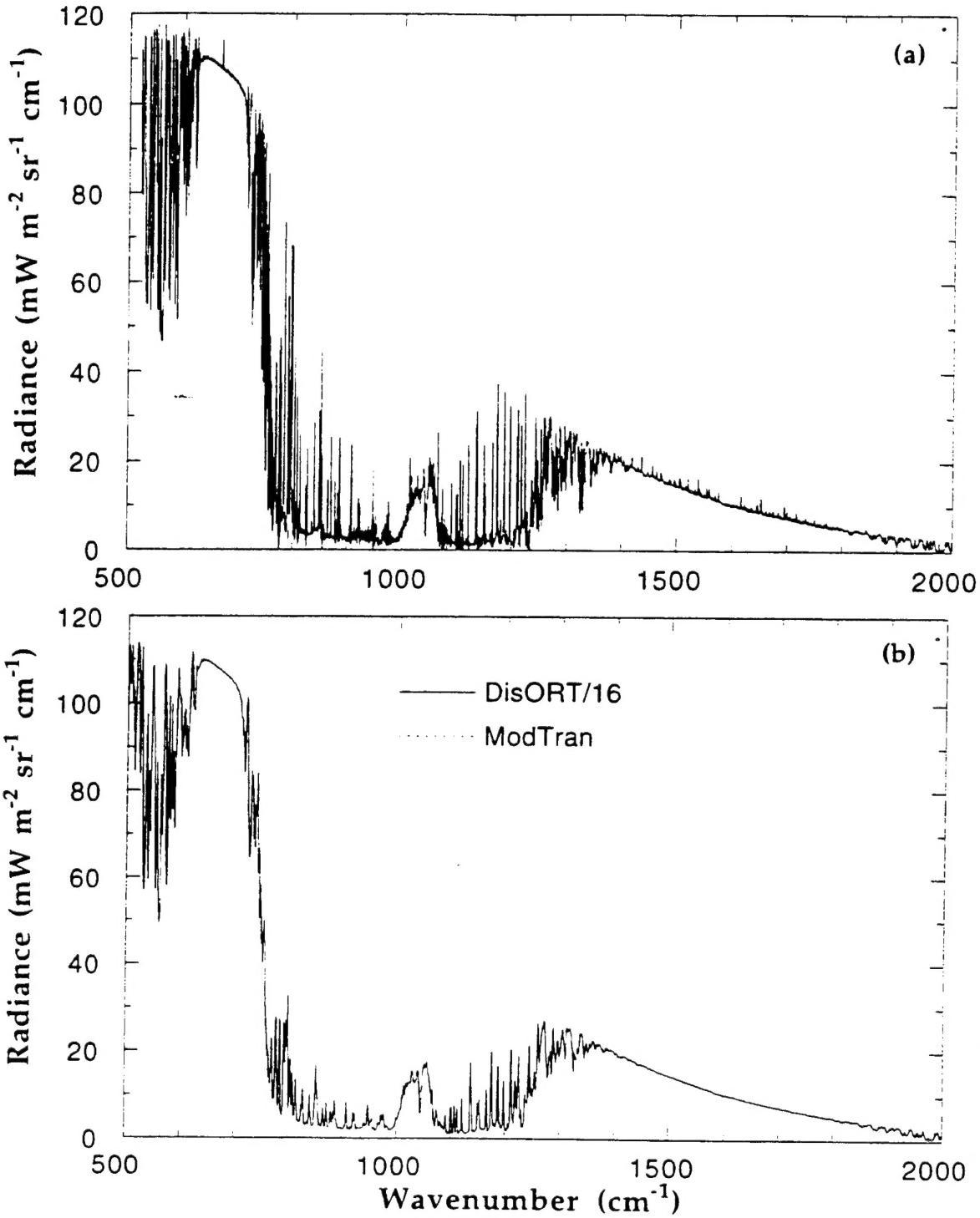

Figure A11. Comparisons of spectral radiance at the surface for (a) measured data, and computed from using (b) merged package with DISORT 16-stream and MODTRAN2 only in the 500 to 2000 cm^{-1} region for a clear atmosphere (see text for details).

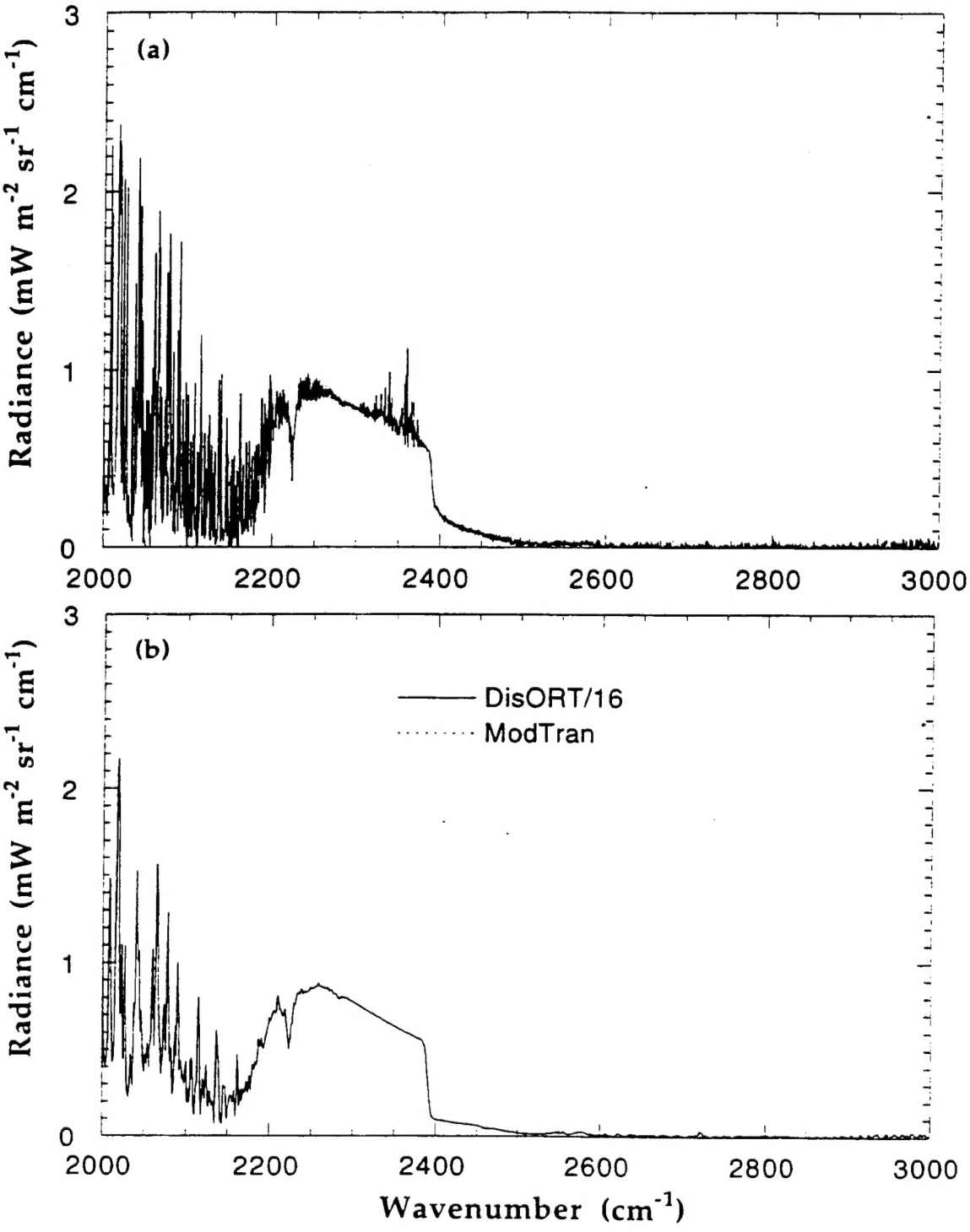

Figure A12. Same as in Figure A11, but for the 2000 to 3000 cm^{-1} (see text for details).

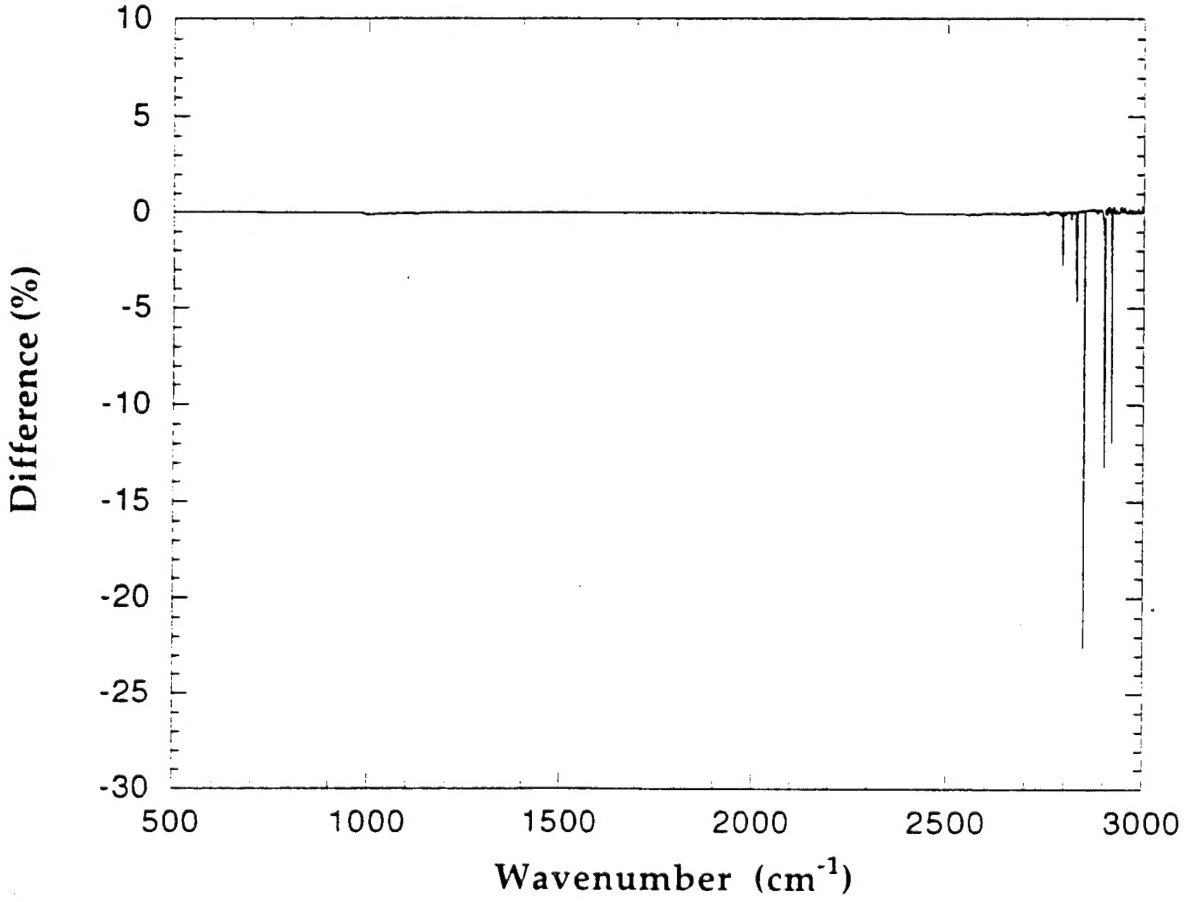

Figure A13. Difference of results between MODTRAN2 and merged package with DISORT 16-stream(see text for details).